O 113: 2D materials beyond graphene: TMDCs, silicene and relatives V

Time: Friday 10:30–13:00 Location: MA 043

O 113.1 Fri 10:30 MA 043

Growth and electronic structure of Sb bilayers on Bi2Se3: a route to achieve buckled antimonene — •Sanjoy K. Mahatha[1,2], Kris Holtgrewe[3], Roberto Flammini[4], Conor Hogan[4], Marco Papagno[5], Alessandro Barla[1], Paolo Moras[1], Polina M. Sheverdyaeva[1], Stefano Colonna[4], Fabio Ronci[4], Simone Sanna[3], Ziya S. Aliev[6], Evgueni V. Chulkov[7], and Carlo Carbone[1] — [1]CNR-ISM, I-34149 Trieste, Italy — [2]Aarhus University, 8000 Aarhus C, Denmark — [3]University of Giessen, Germany — [4]CNR-ISM, I-00133 Roma, Italy — [5]Universita della Calabria, 87036 Arcavacata di Rende (CS), Italy — [6]Azerbaijan National Academy of Science, AZ1143 Baku, Azerbaijan — [7]Donostia International Physics Center, Basque Country, Spain

Hetero-structures consisting of topological insulators and two-dimensional (2D) materials represent an interesting system, where interfacial phenomena play a crucial role, thus allowing for innovative applications. Here, we will give a detailed account of the electronic and atomic structure of Sb bilayers on the Bi2Se3 surface, which has been investigated using scanning tunneling microscopy (STM), angle-resolved photoemission spectroscopy (ARPES) and ab-initio calculations. Our STM results univocally prove the wetting structure of Sb on Bi2Se3 with buckled honeycomb structure. ARPES measurements and calculated band structures show that the hybridization of Sb states with the Bi2Se3 substrate plays an important role in determining the spin-pattern of the surface localized electronic states.

O 113.2 Fri 10:45 MA 043

k-space indirect interlayer excitons in MoS_2/WSe_2 van der Waals heterostructures — •J. Kunstmann[1], F. Mooshammer[2], P. Nagler[2], A. Chaves[3,4], F. Stein[1], N. Paradiso[2], G. Plechinger[2], C. Strunk[2], C. Schüller[2], G. Seifert[1], D. R. Reichman[4], and T. Korn[1] — [1]TU Dresden, DE — [2]Universität Regensburg, DE — [3]Universidade Federal do Ceara, BRA — [4]Columbia University, USA

In heterobilayers of transition metal dichalcogenides (TMDCs) a new type of exciton emerges, where electron and hole are spatially separated. These interlayer excitons allow exploration of many-body quantum phenomena and are ideally suited for valleytronic applications. Mostly, a basic model of fully spatially-separated electron and hole stemming from the K valleys of the monolayer Brillouin zones is applied to describe such excitons. Here, we combine photoluminescence spectroscopy and first principle calculations to expand the concept of interlayer excitons. We identify a partially charge-separated electron-hole pair in MoS_2/WSe_2 heterostructures residing at the Γ and K valleys. We control the emission energy of this new type of k-space indirect, yet strongly-bound exciton by variation of the relative twist angle. These findings represent a crucial step towards the understanding and control of excitonic effects in TMDC heterostructures and devices.

O 113.3 Fri 11:00 MA 043

Material Realistic Description of Coulomb Engineered Two-dimensional Materials — •Christina Steinke[1,2], Malte Rösner[3], Dmitry Ryndyk[2], and Tim Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089-0484, USA

Heterojunctions are building blocks of various applications in modern optoelectronics. Common heterojunctions rely on interfaces of different materials in order to gain the desired spatial band-gap modulations. We investigate a new type of lateral heterojunction imprinted externally into an otherwise homogeneous monolayer of a 2d material. In 2d semiconductors the Coulomb interaction can modify band gaps on an eV scale and can be drastically manipulated by external screening. This allows to tune the local band gaps within a monolayer by laterally structured dielectric surroundings and leads to characteristics of a heterojunction in the local density of states with a spatially sharp band gap modulation. By means of ab-initio calculations we study the nature and tunability of this band-gap modulation in 2d semiconductors in dependence of the chosen environment. Therefore we place a homogeneous monolayer on different laterally structured substrates. We identify optimal candidates for Coulomb engineered 2d systems and study their electronic transport properties depending on external electrical fields and charge doping.

O 113.4 Fri 11:15 MA 043

Strain-induced Formation of Grain Boundaries in the 2D Quantum Spin Hall State in WSe_2 — •Charlotte Herbig[1], Zahra Pedramrazi[1], Madeleine Philips[2], Dillon Wong[1], Yi Chen[1], Hsin-Zon Tsai[1], Shujie Tang[3], Hyejin Ryu[4], Artem Pulkin[5], Zahid Hussain[4], Sung-Kwan Mo[4], Zhi-Xun Shen[3], Oleg Yazyev[5], Eugene Mele[2], and Michael F. Crommie[1] — [1]University of California Berkeley — [2]University of Pennsylvania — [3]Stanford University — [4]Lawrence Berkeley National Lab — [5]École Polytechnique Fédérale de Lausanne

Monolayers of group VI transition metal dichalcogenides with chemical formula MX_2, where M stands for Mo or W and X is S, Se, or Te, come in different structural polymorphs such as 1H, 1T, and 1T'. The metastable 1T' phase of WSe_2 hosts exotic physical properties such as the existence of a 2D topologically non-trivial quantum spin Hall state. The low-symmetry 1T' phase is structurally degenerate and has three orientation variants. Using the atomically sharp tip of a scanning tunneling microscope, we induce strain on monolayer islands of 1T'-WSe_2 and thereby switch between these three orientations, creating and rearranging grain boundaries between two topologically non-trivial 1T' phases. The electronic structure of these grain boundaries is then explored via scanning tunneling spectroscopy and compared with calculations of confined electronic modes on the grain boundary.

O 113.5 Fri 11:30 MA 043

Probing the band structure of quasi-freestanding monolayer MoS_2 — •Clifford Murray[1], Wouter Jolie[1,2], Joshua Hall[1], Carsten Busse[1,2,3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster — [3]Department Physik, Universität Siegen

We epitaxially grow high-quality molybdenum disulfide (MoS_2) monolayers on graphene on Ir(111), and probe its electronic structure with low temperature scanning tunnelling spectroscopy (STS).

A bandgap of 2.50 ± 0.05 eV is measured by STS, showing the freestanding nature of MoS_2 on this substrate. Furthermore, by combining constant height and constant current STS modes and measuring the state-resolved tunnelling decay constant [1], we are able to disentangle the contributions of states located at various high-symmetry points, such as the spin-split valence band at the K-point. The band structure is found to be in close agreement with theoretical calculations for freestanding MoS_2, further evidencing the weak coupling with its Gr/Ir(111) substrate. Additionally, the valence band is seen to undergo a stepwise bending towards twin boundary line defects in the MoS_2 layer - to the best of our knowledge a phenomenon not yet reported in this material.

[1] Zhang, C. et al, Nano Lett. 15, 6494 (2015)

O 113.6 Fri 11:45 MA 043

Evolution of defects in two-dimensional $MoTe_2$: from point to extended defects — •Mahdi Ghorbani-Asl[1], Tibor Lehnert[2], Janis Köster[2], Hannu-Pekka Komsa[3], Ute Kaiser[2], and Arkady Krasheninnikov[1,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Electron Microscopy Group of Materials Science, University of Ulm, Ulm 89081, Germany — [3]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland

Defects frequently govern the characteristics of solids, e.g., mechanical or optical properties. They also provide an efficient way to engineer materials properties, similar to doping in semiconductors. Using first-principles calculations combined with high-resolution transmission electron microscopy experiments, we study creation, agglomeration, and evolution of vacancies in monolayer $MoTe_2$ under electron irradiation. Various types of point and extended defects are studied and their atomic structures and formation energies are determined. The stability of flower-like defects and trefoil-like defects are compared with the line vacancies. Our results show that single Te vacancies have

a tendency for agglomeration into vacancy lines. The stability of line defects is also found to be dependent on their orientation. We have also studied the effects of uniaxial and biaxial strain on the stability and dynamics of line defects. Our electronic structure calculations show that the defects can change the electronic properties of $MoTe_2$, suggesting new opportunities for defect engineering in these layered materials.

O 113.7 Fri 12:00 MA 043

Insights into ferecrystalline layered heterostructures using surface science techniques — •Fabian Göhler[1], Niels Rösch[1], Erik Hadland[2], Danielle Hamann[2], Florian Speck[1], David C. Johnson[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene, Oregon 97403, United States

The stacking of single sheets of 2D materials to design hybrids with new emergent properties is a rapidly emerging field in materials science. An interesting avenue to synthesize a large number of different layered heterostructures on a wafer scale is provided by the Modulated Elemental Reactants (MER) technique, which allows independent control over constituents and layering sequence. $[MX_{1+\delta}]_m[TX_2]_n$ ferecrystal heterostructures are nanocrystalline, turbostratically disordered, layered materials that are synthesized by MER from structurally modulated, amorphous precursors at relatively low temperatures.

The talk will give an overview over recent results obtained from surface science techniques, mainly X-ray photoelectron spectroscopy (XPS) and LEED, on a number of ferecrystal compounds. These techniques provide insight into electronic interactions and structural modulations within and in between distinct layers. Among the results shown are interlayer charge transfer in $[PbSe_{1+\delta}]_1[NbSe_2]_2$ and $[SnSe_{1+\delta}]_m[TiSe_2]_2$, antiphase boundaries in rocksalt-like BiSe bilayers separated by $NbSe_2$ or $MoSe_2$, and structural polytypism in single layers of $MoSe_2$ separated by BiSe.

O 113.8 Fri 12:15 MA 043

Lateral and Vertical Heterostructures of h-GaN/h-AlN: Electron Confinement, Band Lineup, and Quantum Structures — •Engin Durgun, Abdullatif Onen, Deniz Kecik, and Salim Ciraci — Bilkent University - UNAM, Bilkent Ankara Turkey

Lateral and vertical heterostructures constructed of 2D h-GaN and h-AlN display novel electronic and optical properties and diverse quantum structures to be utilized in 2D device applications. Lateral heterostructures formed by periodically repeating narrow h-GaN and h-AlN stripes, which are joined commensurately, behave as composite semiconducting materials. Direct-indirect characters of the band gaps and their values vary with the widths of these stripes. However, for relatively wider stripes, electronic states are confined in different stripes and make a semiconductor-semiconductor junction with normal band alignment. This way 1D multiple quantum well structures can be generated with electrons and holes confined to h-GaN stripes. Vertical heterostructures formed by thin stacks of h-GaN and h-AlN are composite semiconductors with a tunable fundamental band gap. However, depending on the stacking sequence and number of constituent sheets in the stacks, the vertical heterostructure can transform into a junction, which displays staggered band alignment with electrons and holes separated in different stacks. Despite the complexities due to confinement effects, the band diagram of the heterostructures and band lineup are conveniently revealed from the electronic structure projected to the atoms or layers. Prominent features in the optical spectra of the lateral composite structures are observed.

O 113.9 Fri 12:30 MA 043

Nanoscale energy flow in 2D metal / 2D semiconductor heterostructures studied with femtosecond electron diffraction — •Thomas Vasileiadis, Daniela Zahn, Yingpeng Qi, and Ralph Ernstorfer — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin, Germany

Having techniques for studying energy flow mechanisms in systems with nanoscale heterogeneities is essential for the development of future nanodevices. This task can be carried out using femtosecond electron diffraction (FED), a technique in which the lattice response to electronic excitations is probed by ultrashort electron bunches [1]. In this talk we will present FED studies of a 2D metal / 2D semiconductor heterostructure. Our samples consist of exfoliated multilayer flakes of WSe_2 with epitaxially grown Au on their surface. WSe_2 in contact with nanostructured Au is a promising material for optoelectronics. As an example, a recent study reported 20,000-fold enhancement of photoluminescence [2]. For a deeper understanding of energy flow in this system we have studied the laser-induced vibrational excitation of the individual materials by means of the Debye-Waller effect. Our results show that decoration with Au has significant effect on the optical properties and lattice dynamics of WSe_2.

[1] L. Waldecker, R. Bertoni, R. Ernstorfer, J. Appl. Phys. 117, 044903 (2015).

[2] Z Wang, et al. Nature Communications 7, 11283 (2016).

O 113.10 Fri 12:45 MA 043

Structural prediction of two-dimensional materials under strain — •Pedro Borlido[1], Conrad Steigemann[2], Nektarios Lathiotakis[3], Claudia Rödl[1], Miguel Marques[2], and Silvana Botti[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, GR-11635 Athens, Greece

Using a constrained global structural prediction method we performed an extensive investigation of the low density phases of two-dimensional carbon and silicon. As expected, we find that graphene is stable for a large range of biaxial strains, while more complex configurations becoming energetically more favorable at areas per atom above 3.12 $Å^2$. Two dimensional silicon presents a more complex phase diagram, which includes both haeckelite-like structures and dumbbell configurations. In particular, we find as the groundstate of two-dimensional silicon a novel structure formed by a honeycomb lattice with a few strategically positioned dumbbell atoms. This material is 218 meV/atom more stable than silicene and is a quasi-direct semiconductor with a band gap of around 1.11 eV and a very dispersive electron band. These properties should make it easier to synthesize than pristine silicene and interesting for a wealth of opto-electronic applications.